

COMPUTATION OF POLARIZED METRIZED GRAPH INVARIANTS BY USING DISCRETE LAPLACIAN MATRIX

ZUBEYIR CINKIR

ABSTRACT. Several invariants of polarized metrized graphs and their applications in Arithmetic Geometry are studied recently. In this paper, we give fast algorithms to compute these invariants by expressing them in terms of the discrete Laplacian matrix and its pseudo inverse. Algorithms we give can be used for both symbolic and numerical computations. We present various examples to illustrate the implementation of these algorithms.

1. INTRODUCTION

Let X be a geometrically connected curve of genus $\bar{g} \geq 2$ over a field k . Suppose k is either a number field or the function field of a smooth projective curve Y over a field. Assume that X has a semistable model \mathcal{X} over SS , where $SS = \text{Spec} \mathcal{O}_k$ if k is a number field and $SS = Y$ if k is a function field. Let $N(v)$ be the local factor related to the product formula for k . In this context, $\omega_{\mathcal{X}/SS}^2$, the self intersection of the relative dualizing sheaf $\omega_{\mathcal{X}/SS}$, is an important quantity both in geometric and arithmetic case. Lower and upper bounds to this quantity are of interest in diophantine geometry.

In 1993, Zhang [24] expressed $\omega_{\mathcal{X}/SS}^2$ in terms of ω_a^2 , the self intersection of the admissible relative dualizing sheaf ω_a associated to a minimal regular model of X :

$$(1) \quad \omega_{\mathcal{X}/SS}^2 = \omega_a^2 + \sum_v \epsilon(X_v) \log N(v),$$

where v runs over the set of non-archimedean places of k , and $\epsilon(X_v)$ is a certain local invariant of the reduction graph $R(X_v)$ associated to the completion of X at a place v of k .

In 2010, Zhang [25, Corollary 1.3.2] expressed ω_a^2 in terms of $\langle \Delta_\xi, \Delta_\xi \rangle$, the arithmetic self intersection (equal to the canonical height) of the Gross-Schoen cycle $\Delta_\xi \subset X \times X \times X$:

$$(2) \quad \omega_a^2 = \frac{2\bar{g}-2}{2\bar{g}+1} \langle \Delta_\xi, \Delta_\xi \rangle + \frac{2\bar{g}-2}{2\bar{g}+1} \sum_v \varphi(X_v) \log N(v),$$

where v runs over the set of places of k , and $\varphi(X_v)$ is a certain local invariant again linked to the reduction graph $R(X_v)$ at each place v of k .

On the other hand, we have the following equality for a semistable fibration $f : \mathcal{X} \rightarrow SS$ by Nother's formula:

$$(3) \quad \omega_{\mathcal{X}/SS}^2 = 12 \deg f_*(\omega_{\mathcal{X}/SS}) - \sum_v \delta(X_v),$$

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where $\delta(X_v)$ is the total number of the singular points in the fiber over v . Moreover, Zhang [25] showed that

$$(4) \quad \deg f_*(\omega_{X/SS}) = \frac{\bar{g} - 1}{6(2\bar{g} + 1)} \langle \Delta_\xi, \Delta_\xi \rangle + \sum_v \lambda(X_v) \log N(v),$$

where v runs over the set of places of k , and $\lambda(X_v)$ is another local invariant associated to the reduction graphs $R(X_v)$. We refer [14] for other connections between $\lambda(X_v)$ and some invariants of complex moduli space of curves of genus higher than 1.

Whenever v is a non-archimedean place, the local invariants $\varphi(X_v)$, $\epsilon(X_v)$, $\lambda(X_v)$ are defined as the invariants of the corresponding polarized metrized graph. Note that the reduction graph $R(X)$ of any semistable curve X of genus \bar{g} over a discrete valuation ring is a polarized metrized graph of genus \bar{g} .

We also have invariants $Z(\Gamma)$, $\tau(\Gamma)$ and $\theta(\Gamma)$ (see §2 below) of a polarized metrized graph Γ , which are closely related to the local invariants given above.

Explicit computations of these local invariants were done only for some curves of genus less than or equal to 4 (see [17], [18], [11], [21], [22], [23], [13], [5]). Other than some families of polarized metrized graph of certain types, explicit computations become a huge intricate task for a person as soon as \bar{g} gets larger than 3. Thus, one needs a computer algorithm to do such computations. We have such an algorithm to compute $\tau(\Gamma)$ (see [5] and [9]). Also, X. Faber gave an algorithm to compute the invariants $\epsilon(\Gamma)$, $\varphi(\Gamma)$, $\lambda(\Gamma)$ and $Z(\Gamma)$ (see [11] and [12]).

In this paper, we provide a fast computer algorithm that can be used for both symbolic and numeric computation of each of the polarized metrized graph invariants. This algorithm is faster, because it takes advantage of two important facts: All of the effective resistance computations can be handled by just one matrix inversion (see Equation (11) and Lemma 3.2), and the computations of the invariants $\epsilon(\Gamma)$, $\varphi(\Gamma)$, $\lambda(\Gamma)$ and $Z(\Gamma)$ can be reduced to the computations of $\tau(\Gamma)$ and $\theta(\Gamma)$ (see Theorem 2.3).

In §2, we give a short revision of a polarized metrized graph and definitions of its invariants (see Lemma 2.1, Equation (8) and Equation (9)). Using Theorem 2.3, the problem of computing the invariants $\epsilon(\Gamma)$, $\varphi(\Gamma)$, $\lambda(\Gamma)$ and $Z(\Gamma)$ are reduced to the computations of $\tau(\Gamma)$ and $\theta(\Gamma)$. Using these connections and our previous results about $\tau(\Gamma)$ and $\theta(\Gamma)$, we explain how to deal with self loops and multiple edges, if desired, as the initial step of the algorithm.

In §3, we define discrete Laplacian matrices associated to polarized metrized graphs. We express $\theta(\Gamma)$ in terms of the discrete Laplacian matrix L and its pseudo inverse L^+ (see Theorem 3.6). Then we use our previous result on $\tau(\Gamma)$ to express the invariants $\epsilon(\Gamma)$, $\varphi(\Gamma)$, $\lambda(\Gamma)$ and $Z(\Gamma)$ in terms of the entries of L and L^+ . This gives us the main result in this paper. Namely, each of these invariants can be symbolically or numerically computed with the algorithm we provide.

Finally, we give various examples to show the implementation of our algorithm in §4.

2. POLARIZED METRIZED GRAPHS AND THEIR INVARIANTS

In this section, we first give brief descriptions of a metrized graph Γ , a polarized metrized graph (Γ, \mathbf{q}) , invariants $\tau(\Gamma)$, $\theta(\Gamma)$, $\epsilon(\Gamma)$, $\varphi(\Gamma)$, $\lambda(\Gamma)$ and $Z(\Gamma)$ associated to (Γ, \mathbf{q}) .

A metrized graph Γ is a finite connected graph equipped with a distinguished parametrization of each of its edges. A metrized graph Γ can have multiple edges and self-loops. For any given $p \in \Gamma$, the number $v(p)$ of directions emanating from p will be called the *valence* of p . By definition, there can be only finitely many $p \in \Gamma$ with $v(p) \neq 2$.

For a metrized graph Γ , we will denote a vertex set for Γ by $V(\Gamma)$. We require that $V(\Gamma)$ be finite and non-empty and that $p \in V(\Gamma)$ for each $p \in \Gamma$ if $v(p) \neq 2$. For a given metrized graph Γ , it is possible to enlarge the vertex set $V(\Gamma)$ by considering additional valence 2 points as vertices.

For a given metrized graph Γ with vertex set $V(\Gamma)$, the set of edges of Γ is the set of closed line segments with end points in $V(\Gamma)$. We will denote the set of edges of Γ by $E(\Gamma)$. However, if e_i is an edge, by $\Gamma - e_i$ we mean the graph obtained by deleting the *interior* of e_i .

We define the genus of Γ to be the first Betti number $g(\Gamma) := e - v + 1$ of the graph Γ , where e and v are the number of edges and vertices of Γ , respectively.

We denote the length of an edge $e_i \in E(\Gamma)$ by L_i , which represents a positive real number. The total length of Γ , which is denoted by $\ell(\Gamma)$, is given by $\ell(\Gamma) = \sum_{i=1}^e L_i$.

If a metrized graph Γ is viewed as a resistive electric circuit with terminals at x and y , with the resistance in each edge given by its length, then $r(x, y)$ is the effective resistance between x and y when unit current enters at y and exits at x .

For any x, y in Γ , the resistance function $r(x, y)$ on Γ is a symmetric function in x and y , and it satisfies $r(x, x) = 0$. For each vertex set $V(\Gamma)$, $r(x, y)$ is continuous on Γ as a function of two variables and $r(x, y) \geq 0$ for all x, y in Γ . For proofs of these facts and connections between the resistance function and the voltage function on Γ , see articles [10], [2, sec 1.5 and sec 6], and [24, Appendix]. The resistance function $r(x, y)$ on a metrized graph were also studied in the articles [1] and [6].

We will denote by $R_i(\Gamma)$, or by R_i if there is no danger of confusion, the resistance between the end points of an edge e_i of a graph Γ when the interior of the edge e_i is deleted from Γ .

The tau constant $\tau(\Gamma)$ of a metrized graph Γ was initially defined by Baker and Rumely [2, Section 14]. The following lemma gives a description of the tau constant. In particular, it implies that the tau constant is positive.

Lemma 2.1. [2, Lemma 14.4] *For any fixed y in Γ , $\tau(\Gamma) = \frac{1}{4} \int_{\Gamma} \left(\frac{\partial}{\partial x} r(x, y) \right)^2 dx$.*

One can find more detailed information on $\tau(\Gamma)$ in articles [5], [6], [7] and [9].

On a metrized graph Γ , we have a *canonical measure* μ_{can} first studied by Chinburg and Rumely [10]. See the articles [2] and [6] for several interpretations of μ_{can} . The following theorem gives an explicit description of μ_{can} :

Theorem 2.2. [10, Theorem 2.11] *For a given metrized graph Γ , let L_i and R_i be defined as before. Then we have*

$$\mu_{\text{can}}(x) = \sum_{p \in V(\Gamma)} \left(1 - \frac{1}{2}v(p)\right) \delta_p(x) + \sum_{e_i \in E(\Gamma)} \frac{dx}{L_i + R_i}.$$

Let Γ be a metrized graph and let $\mathbf{q} : \Gamma \rightarrow \mathbb{N}$ be a function supported on the set of vertices of Γ . The canonical divisor K of (Γ, \mathbf{q}) is defined to be the following divisor on Γ :

$$(5) \quad K = \sum_{p \in V(\Gamma)} (v(p) - 2 + 2\mathbf{q}(p))p, \quad \text{and} \quad \delta_K(x) = \sum_{p \in V(\Gamma)} (v(p) - 2 + 2\mathbf{q}(p))\delta_p(x).$$

The pair (Γ, \mathbf{q}) is called a *polarized metrized graph* (pm-graph in short) if \mathbf{q} is non-negative and K is an effective divisor. Whenever $\mathbf{q} = 0$, (Γ, \mathbf{q}) is called a simple pm-graph. The

genus $\bar{g}(\Gamma)$ of a pm-graph (Γ, \mathbf{q}) is defined to be

$$(6) \quad \bar{g}(\Gamma) = 1 + \frac{1}{2} \deg K = g(\Gamma) + \sum_{p \in V(\Gamma)} \mathbf{q}(p).$$

We will simply use \bar{g} instead of $\bar{g}(\Gamma)$ when there is no danger of confusion.

Let $\mu_{ad}(x)$ be the admissible measure associated to K (defined by Zhang [24, Lemma 3.7]). We have

$$\mu_{ad}(x) = \frac{1}{\bar{g}} \left(\sum_{p \in V(\Gamma)} \mathbf{q}(p) \delta_p(x) + \sum_{e_i \in E(\Gamma)} \frac{dx}{L_i + R_i} \right).$$

Then, if we use Theorem 2.2, we can relate $\mu_{ad}(x)$ and $\mu_{can}(x)$ as follows:

$$(7) \quad \mu_{ad}(x) = \frac{1}{2\bar{g}} (2\mu_{can}(x) + \delta_K(x)).$$

Moreover, $\delta_K(\Gamma) = \deg(K) = 2\bar{g} - 2$, and we have $\mu_{can}(\Gamma) = 1 = \mu_{ad}(\Gamma)$.

On a pm-graph (Γ, \mathbf{q}) , we defined and studied ([5] and [8]) the invariant $\theta(\Gamma)$ as follows:

$$(8) \quad \theta(\Gamma) := \sum_{p, q \in V(\Gamma)} (v(p) - 2 + 2\mathbf{q}(p))(v(q) - 2 + 2\mathbf{q}(q))r(p, q).$$

We have $\theta(\Gamma) \geq 0$ for any pm-graph Γ , since the canonical divisor K is effective.

Now, we can give definitions of the invariants $\epsilon(\Gamma)$, $\varphi(\Gamma)$, $\lambda(\Gamma)$ and $Z(\Gamma)$ (c.f. [25, Section 4.1]) of Γ :

$$(9) \quad \begin{aligned} \epsilon(\Gamma) &= \iint_{\Gamma \times \Gamma} r(x, y) \delta_K(x) \mu_{ad}(x), & Z(\Gamma) &= \frac{1}{2} \iint_{\Gamma \times \Gamma} r(x, y) \mu_{ad}(x) \mu_{ad}(y), \\ \varphi(\Gamma) &= 3\bar{g} \cdot Z(\Gamma) - \frac{1}{4}(\epsilon(\Gamma) + \ell(\Gamma)), & \lambda(\Gamma) &= \frac{\bar{g} - 1}{6(2\bar{g} + 1)} \varphi(\Gamma) + \frac{1}{12}(\epsilon(\Gamma) + \ell(\Gamma)). \end{aligned}$$

We can express invariants given in Equation (9) in terms of $\tau(\Gamma)$ and $\theta(\Gamma)$ ([8, Propositions 4.6, 4.7, 4.9 and Theorem 4.8]):

Theorem 2.3. *Let (Γ, \mathbf{q}) be a pm-graph. Then we have*

$$\begin{aligned} \varphi(\Gamma) &= \frac{(5\bar{g} - 2)\tau(\Gamma)}{\bar{g}} + \frac{\theta(\Gamma)}{4\bar{g}} - \frac{\ell(\Gamma)}{4}, & Z(\Gamma) &= \frac{(2\bar{g} - 1)\tau(\Gamma)}{\bar{g}^2} + \frac{\theta(\Gamma)}{8\bar{g}^2}, \\ \lambda(\Gamma) &= \frac{(3\bar{g} - 3)\tau(\Gamma)}{4\bar{g} + 2} + \frac{\theta(\Gamma)}{16\bar{g} + 8} + \frac{(\bar{g} + 1)\ell(\Gamma)}{16\bar{g} + 8}, & \epsilon(\Gamma) &= \frac{(4\bar{g} - 4)\tau(\Gamma)}{\bar{g}} + \frac{\theta(\Gamma)}{2\bar{g}}. \end{aligned}$$

Remark 2.4. *Given a pm-graph (Γ, \mathbf{q}) and $s \in \Gamma - V(\Gamma)$, we have $\mathbf{q}(s) = 0$ and $v(s) = 2$. If we enlarge the vertex set by considering s as a vertex with the same \mathbf{q} value on s , $\theta(\Gamma)$ does not change. We recall that this process also does not change the value of $\tau(\Gamma)$ (the valence property of $\tau(\Gamma)$, see [6, Remark 2.10]). Conversely, if $\mathbf{q}(s) = 0$ and $v(s) = 2$ for some $s \in V(\Gamma)$ with $V(\Gamma)$ has at least two elements, then removing s from the vertex set of Γ does not change $\tau(\Gamma)$ and $\theta(\Gamma)$ (such vertices are called eliminable vertices in [21, pg. 152]). Using these observations along with Theorem 2.3, we note that $\epsilon(\Gamma)$, $Z(\Gamma)$, $\varphi(\Gamma)$ and $\lambda(\Gamma)$ do not change under this process. That is, each of these invariants has the valence property.*

Let (Γ, \mathbf{q}) be a polarized metrized graph containing a self loop of length L at a vertex p with $v(p) \geq 3$. Let β be a metrized graph obtained from Γ by deleting this self loop. We still have $p \in V(\beta)$ but its valence is reduced by 2. Now, we consider a function $\bar{\mathbf{q}} : \beta \rightarrow \mathbb{N}$ supported on the set of vertices of β that satisfies $\bar{\mathbf{q}}(p) = \mathbf{q}(p) + 1$ and $\bar{\mathbf{q}}(x) = \mathbf{q}(x)$ for

every $x \in \beta - \{p\}$. Note that $(\beta, \bar{\mathbf{q}})$ is a polarized metrized graph, and that $\bar{g}(\Gamma) = \bar{g}(\beta)$, $\ell(\Gamma) = \ell(\beta) + L$, $\theta(\Gamma) = \theta(\beta)$ and $\tau(\Gamma) = \tau(\beta) + \frac{L}{12}$ by the additive property of $\tau(\Gamma)$ [6, pg. 15] and by the fact that a self loop of length L has the tau constant value $\frac{L}{12}$. Using these facts along with Theorem 2.3, we obtain the following equalities:

$$(10) \quad \begin{aligned} \varphi(\Gamma) &= \varphi(\beta) + \frac{\bar{g} - 1}{6\bar{g}}L, & Z(\Gamma) &= Z(\beta) + \frac{2\bar{g} - 1}{12\bar{g}^2}L, \\ \lambda(\Gamma) &= \lambda(\beta) + \frac{\bar{g}}{8\bar{g} + 4}L, & \epsilon(\Gamma) &= \epsilon(\beta) + \frac{\bar{g} - 1}{3\bar{g}}L. \end{aligned}$$

Successive application of the process above gives a pm-graph β that is either a graph with one vertex and a self loop at this vertex or a graph without self loops. For the first case, we can use the following proposition (part of which is nothing but [25, Proposition 4.4.3]. Here we give a new proof.):

Proposition 2.5. *Let (Γ, \mathbf{q}) be a pm-graph with one vertex and $e \geq 1$ self loops at its vertex. Then*

$$\begin{aligned} \varphi(\Gamma) &= \frac{\bar{g} - 1}{6\bar{g}}\ell(\Gamma), & Z(\Gamma) &= \frac{2\bar{g} - 1}{12\bar{g}^2}\ell(\Gamma), \\ \lambda(\Gamma) &= \frac{\bar{g}}{8\bar{g} + 4}\ell(\Gamma), & \epsilon(\Gamma) &= \frac{\bar{g} - 1}{3\bar{g}}\ell(\Gamma). \end{aligned}$$

Proof. If Γ has just one self loop, then $\tau(\Gamma) = \frac{\ell(\Gamma)}{12}$ and $\theta(\Gamma) = 0$. Thus, the result follows from Theorem 2.3 in this case. Applying the procedure given in Equation (10), one can show that the result still holds if Γ has more than one self loop. \square

Hence, we can focus on pm-graphs with no self loop.

3. DISCRETE LAPLACIAN

In this section, we first describe the discrete Laplacian matrix of a finite weighted graph with no self loops and multiple edges. Then following [9], we define discrete Laplacian matrices associated to a metrized graph Γ and a pm-graph (Γ, \mathbf{q}) . Then we express invariants of a pm-graph in terms of the associated discrete Laplacian matrices, their pseudo inverse and values of \mathbf{q} . This enables us to achieve our main goal in this paper. Namely, we derive a feasible algorithm for both numeric and symbolic computations of pm-graph invariants.

To have a well-defined discrete Laplacian matrix L for a metrized graph Γ , we first choose a vertex set $V(\Gamma)$ for Γ in such a way that there are no self-loops, and no multiple edges connecting any two vertices. This can be done by enlarging the vertex set by considering additional valence two points as vertices whenever needed. We call such a vertex set $V(\Gamma)$ *adequate*. If distinct vertices p and q are the end points of an edge, we call them *adjacent* vertices.

Let Γ be a metrized graph with e edges and an adequate vertex set $V(\Gamma)$ containing v vertices. Fix an ordering of the vertices in $V(\Gamma)$. Let $\{L_1, L_2, \dots, L_e\}$ be a labeling of the edge lengths. The matrix $A = (a_{pq})_{v \times v}$ given by

$$a_{pq} = \begin{cases} 0, & \text{if } p = q, \text{ or } p \text{ and } q \text{ are not adjacent.} \\ \frac{1}{L_k}, & \text{if } p \neq q, \text{ and an edge of length } L_k \text{ connects } p \text{ and } q. \end{cases}$$

is called the *adjacency matrix* of Γ . Let $D = \text{diag}(d_{pp})$ be the $v \times v$ diagonal matrix given by $d_{pp} = \sum_{s \in V(\Gamma)} a_{ps}$. Then $L := D - A$ is called the *discrete Laplacian matrix* of Γ . That

is, $L = (l_{pq})_{v \times v}$ where

$$l_{pq} = \begin{cases} 0, & \text{if } p \neq q, \text{ and } p \text{ and } q \text{ are not adjacent.} \\ -\frac{1}{L_k}, & \text{if } p \neq q, \text{ and } p \text{ and } q \text{ are connected by an edge of length } L_k. \\ -\sum_{s \in V(\Gamma) - \{p\}} l_{ps}, & \text{if } p = q \end{cases}$$

We define the discrete Laplacian matrix corresponding to pm-graph (Γ, \mathbf{q}) as the discrete Laplacian L corresponding to the metrized graph Γ . Important thing is that if the vertex set of (Γ, \mathbf{q}) is needed to be enlarged to make it an adequate vertex set we set \mathbf{q} value 0 for those new vertices added because of self loops or multiple edges.

Although L is not invertible, it has generalized inverses. In particular, it has the pseudo inverse L^+ , also known as the Moore-Penrose generalized inverse. The pseudo inverse L^+ is uniquely determined by the following properties:

$$\begin{aligned} i) \quad & LL^+L = L, & iii) \quad & (LL^+)^T = LL^+, \\ ii) \quad & L^+LL^+ = L^+, & iv) \quad & (L^+L)^T = L^+L. \end{aligned}$$

For a discrete Laplacian matrix L of size $v \times v$, the following formula for L^+ (see [20, ch 10]) is crucial for our computations:

$$(11) \quad L^+ = \left(L - \frac{1}{v}J\right)^{-1} + \frac{1}{v}J.$$

where J is of size $v \times v$ and has all entries 1.

L and L^+ are symmetric matrices.

Remark 3.1. We have $\sum_{p \in V(\Gamma)} l_{pq} = 0 = \sum_{p \in V(\Gamma)} l_{pq}^+$, for each $q \in V(\Gamma)$.

Lemma 3.2. [3], [4], [15, Theorem A] Suppose Γ is a graph with the discrete Laplacian L and the resistance function $r(x, y)$. For the pseudo inverse L^+ we have

$$r(p, q) = l_{pp}^+ - 2l_{pq}^+ + l_{qq}^+, \quad \text{for any } p, q \in V(\Gamma).$$

It is important that $\tau(\Gamma)$ can be expressed in terms of the discrete Laplacian matrix and its pseudo inverse:

Theorem 3.3. [9, Theorem 4.10] Let L be the discrete Laplacian matrix of size $v \times v$ for a metrized graph Γ , and let L^+ be its Moore-Penrose pseudo inverse. Suppose p_i and q_i are end points of $e_i \in E(\Gamma)$. Then we have

$$\tau(\Gamma) = -\frac{1}{12} \sum_{e_i \in E(\Gamma)} l_{p_i q_i} \left(\frac{1}{l_{p_i q_i}} + l_{p_i p_i}^+ - 2l_{p_i q_i}^+ + l_{q_i q_i}^+ \right)^2 + \frac{1}{4} \sum_{q, s \in V(\Gamma)} l_{qs} l_{qq}^+ l_{ss}^+ + \frac{1}{v} \text{tr}(L^+).$$

Moreover, $\sum_{q, s \in V(\Gamma)} l_{qs} l_{qq}^+ l_{ss}^+ = -\sum_{e_i \in E(\Gamma)} l_{p_i q_i} (l_{p_i p_i}^+ - l_{q_i q_i}^+)^2$.

Similarly, one can express μ_{can} in terms of the discrete Laplacian matrix and its pseudo inverse:

Proposition 3.4. [9, Prop. 4.12] For a given metrized graph Γ , let L be its discrete Laplacian, and let L^+ be the corresponding pseudo inverse. Suppose p_i and q_i are end points of $e_i \in E(\Gamma)$. Then we have

$$\mu_{can}(x) = \sum_{p \in V(\Gamma)} \left(1 - \frac{1}{2}v(p)\right) \delta_p(x) - \sum_{e_i \in E(\Gamma)} (l_{p_i q_i} + l_{p_i q_i}^2 (l_{p_i p_i}^+ - 2l_{p_i q_i}^+ + l_{q_i q_i}^+)) dx.$$

Using Equation (7) and Proposition 3.4, we express $\mu_{ad}(x)$ in terms of the entries of L and L^+ :

Proposition 3.5. *For a given pm-graph (Γ, \mathbf{q}) , let L be its discrete Laplacian, and let L^+ be the corresponding pseudo inverse. Suppose p_i and q_i are end points of $e_i \in E(\Gamma)$. Then we have*

$$\mu_{ad}(x) = \frac{1}{\bar{g}} \sum_{p \in V(\Gamma)} \mathbf{q}(p) \delta_p(x) - \frac{1}{\bar{g}} \sum_{e_i \in E(\Gamma)} (l_{p_i q_i} + l_{p_i q_i}^2 (l_{p_i p_i}^+ - 2l_{p_i q_i}^+ + l_{q_i q_i}^+)) dx.$$

The next important observation is that $\theta(\Gamma)$ can be expressed in terms of L and L^+ :

Theorem 3.6. *Let (Γ, \mathbf{q}) be a pm-graph. Then*

$$\theta(\Gamma) = 2(2\bar{g} - 2) \sum_{p \in V(\Gamma)} (v(p) - 2 + 2\mathbf{q}(p)) l_{pp}^+ - 2 \sum_{p, q \in V(\Gamma)} (v(p) + 2\mathbf{q}(p))(v(q) + 2\mathbf{q}(q)) l_{pq}^+.$$

Proof. Since $\deg(K) = 2\bar{g} - 2$, $\sum_{s \in V(\Gamma)} (v(s) - 2 + 2\mathbf{q}(s)) = 2\bar{g} - 2$. Then the result follows from Equation (8), Lemma 3.2 and Remark 3.1. \square

Whenever $\mathbf{q} = 0$ on Γ , i.e. Γ is a simple graph, we have $\bar{g} = g = e - v + 1$ and

$$(12) \quad \theta(\Gamma) = 2(2g - 2) \sum_{p \in V(\Gamma)} (v(p) - 2) l_{pp}^+ - 2 \sum_{p, q \in V(\Gamma)} v(p) v(q) l_{pq}^+.$$

Moreover, if Γ is both simple and r -regular, we have $e = \frac{r}{2}v$, $\bar{g} = \frac{r-2}{2}v + 1$ and we have

$$(13) \quad \theta(\Gamma) = 2v(r - 2)^2 tr(L^+),$$

since $\sum_{p \in V(\Gamma)} l_{pq}^+ = 0$.

Given a pm-graph (Γ, \mathbf{q}) , we can give the steps of the algorithm to compute the invariants $\epsilon(\Gamma)$, $\varphi(\Gamma)$, $\lambda(\Gamma)$ and $Z(\Gamma)$ as follows:

Set L be the discrete Laplacian matrix corresponding to Γ . (Choose an adequate vertex set so that there will be no self loops or no multiple edges. Alternatively, use Equation (10) for self loops.)

Set v be the number of rows in L (i.e., the number of vertices in Γ).

Set e be the number of nonzero entries above the diagonal of L (i.e., the number of edges in Γ).

Set $\ell(\Gamma)$ be the negative of the sum of the reciprocals of nonzero entries above the diagonal of L (i.e., the total length of Γ).

Compute \bar{g} by using Equation (6).

Compute L^+ , pseudo inverse of L , by using the formula given in Equation (11).

Compute $\tau(\Gamma)$ by using Theorem 3.3.

Define a function v whose value at i is, $v(i)$, the number of nonzero off diagonal entries in the i -th row of L (i.e., $v(i)$ is the valence of the vertex i).

Compute $\theta(\Gamma)$ by using Theorem 3.6.

Compute $\epsilon(\Gamma)$, $\varphi(\Gamma)$, $\lambda(\Gamma)$ and $Z(\Gamma)$ by using Theorem 2.3.

Note that the most costly part of this algorithm is to obtain L^+ from L .

4. EXAMPLES

In this section, we give various examples illustrating the implementation of the algorithm described in the previous section.

A symbolic computation is exemplified as follows:

Example 1:

Let Γ be a simple pm-graph as illustrated in Figure 1. In this case, we have $\ell(\Gamma) = \frac{1}{a} + \frac{1}{b} + \frac{1}{c} + \frac{1}{d} + \frac{1}{e} + \frac{1}{f}$, and the discrete Laplacian matrix corresponding to Γ is given as

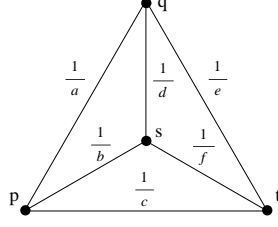


FIGURE 1. Complete graph with vertices $\{p, q, s, t\}$ and edges of lengths $\{\frac{1}{a}, \frac{1}{b}, \frac{1}{c}, \frac{1}{d}, \frac{1}{e}, \frac{1}{f}\}$.

follows:

$$L = \begin{bmatrix} a+b+c & -a & -b & -c \\ -a & a+d+e & -d & -e \\ -b & -d & b+d+f & -f \\ -c & -e & -f & c+e+f \end{bmatrix}.$$

We first compute L^+ by using Equation (11), then use the algorithms given above to derive the following results:

$$\begin{aligned} \tau(\Gamma) &= \frac{1}{12}\ell(\Gamma) - \frac{A+2B}{6C}, & \theta(\Gamma) &= \frac{6A+8B}{C}, \\ \varphi(\Gamma) &= \frac{1}{9}\ell(\Gamma) - \frac{2A+7B}{9C}, & \lambda(\Gamma) &= \frac{3}{28}\ell(\Gamma) + \frac{A}{28C}, \\ Z(\Gamma) &= \frac{5}{108}\ell(\Gamma) - \frac{A+8B}{108C}, & \epsilon(\Gamma) &= \frac{2}{9}\ell(\Gamma) + \frac{5A+4B}{9C}, \end{aligned}$$

where $A = ab + ac + bc + ad + bd + ae + ce + de + bf + cf + df + ef$, $B = cd + be + af$, $C = abc + acd + bcd + abe + bce + ade + bde + cde + abf + acf + adf + bdf + cdf + aef + bef + cef$.

The following example has mostly numeric computations and some symbolic computations because of non-zero \mathbf{q} .

Example 2:

Let Γ be a pm-graph (Γ, \mathbf{q}) such that Γ is the complete graph on 4 vertices $\{p, q, s, t\}$ as in Figure 1. Suppose that each edge of Γ has length $\frac{1}{6}$ and that $\mathbf{q}(p) = \mathbf{q}(q) = \mathbf{q}(s) = \mathbf{q}(t) = k$ for some nonnegative integer k . In this case, we have $\ell(\Gamma) = 1$, the following discrete Laplacian matrix and its pseudo inverse:

$$L = \begin{bmatrix} 18 & -6 & -6 & -6 \\ -6 & 18 & -6 & -6 \\ -6 & -6 & 18 & -6 \\ -6 & -6 & -6 & 18 \end{bmatrix}, \quad L^+ = \begin{bmatrix} \frac{1}{32} & \frac{-1}{96} & \frac{-1}{96} & \frac{-1}{96} \\ \frac{-1}{96} & \frac{1}{32} & \frac{-1}{96} & \frac{-1}{96} \\ \frac{-1}{96} & \frac{-1}{96} & \frac{1}{32} & \frac{-1}{96} \\ \frac{-1}{96} & \frac{-1}{96} & \frac{-1}{96} & \frac{1}{32} \end{bmatrix}.$$

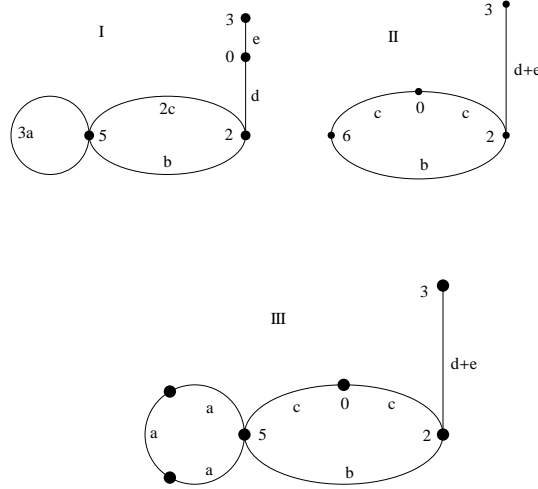
Then we obtain these results:

$$\begin{aligned} \tau(\Gamma) &= \frac{5}{96}, & \theta(\Gamma) &= (1+2k)^2, & \varphi(\Gamma) &= \frac{96k^2 + 100k + 17}{96(4k+3)}, \\ \lambda(\Gamma) &= \frac{16k^2 + 42k + 25}{32(8k+7)}, & Z(\Gamma) &= \frac{48k^2 + 88k + 37}{96(4k+3)^2}, & \epsilon(\Gamma) &= \frac{(12k+11)(2k+1)}{12(4k+3)}. \end{aligned}$$

In particular, if $k = 0$, $\theta(\Gamma) = 1$, $\varphi(\Gamma) = \frac{17}{288}$, $\lambda(\Gamma) = \frac{25}{224}$, $Z(\Gamma) = \frac{37}{864}$ and $\epsilon(\Gamma) = \frac{11}{36}$.

Sometimes we are given pm-graphs containing self loops or multiple edges. We exemplify our strategy for such cases in detail as follows:

Example 3:

FIGURE 2. A pm-graph with a self loop, nonzero \mathbf{q} and two multiple edges.

In this example, we consider a pm-graph (Γ, \mathbf{q}) as the graph *I* in Figure 2, where the edge lengths and the values of \mathbf{q} are illustrated. In this case, Γ has a self loop and two multiple edges. We first ignore the vertex with \mathbf{q} value 0 and valence 2. To avoid having multiple edges, we add a vertex to one of the multiple edges such that the added vertex has \mathbf{q} value 0. We can deal with the self loop by either applying Equation (10) or considering two additional vertex with \mathbf{q} value 0 on the self loop. These cases are illustrated by graphs *II* and *III* in Figure 2. Thus, we can compute polarized metrized graph invariants of Γ in two different ways, and the results are as follows:

$$\begin{aligned} \tau(\Gamma) &= \frac{b + 2c + 3(a + A)}{12}, & \theta(\Gamma) &= \frac{480bc}{b + 2c} + 170A, \\ \varphi(\Gamma) &= \frac{11a}{24} + \frac{11b^2 + 764bc + 44c^2}{72(b + 2c)} + \frac{9A}{2}, & \lambda(\Gamma) &= \frac{9a}{25} + \frac{3(b^2 + 24bc + 4c^2)}{25(b + 2c)} + \frac{27A}{25}, \\ \epsilon(\Gamma) &= \frac{11a}{12} + \frac{11b^2 + 764bc + 44c^2}{36(b + 2c)} + 8A, & Z(\Gamma) &= \frac{23a}{576} + \frac{23b^2 + 812bc + 92c^2}{1728(b + 2c)} + \frac{3A}{16}, \end{aligned}$$

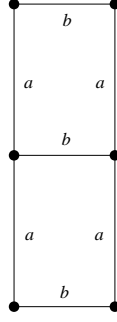
where $A = d + e$, $\ell(\Gamma) = 3a + b + 2c + d + e$, $g(\Gamma) = 2$ and $\bar{g}(\Gamma) = 12$.

The following example is about the computation of invariants of a class of simple pm-graphs. It is given to show both symbolic computations and different aspects of numerical computations which would be critical during the implementation of our algorithm.

Example 4:

A ladder graph $L_n(a, b)$ is planar graph that looks like a ladder with n rungs. It has $2n$ vertices and $3n - 2$ edges. Edges looking like rungs are of lengths b , and each of the remaining $2(n - 1)$ edges has length a . Thus, $\ell(L_n(a, b)) = 2(n - 1)a + nb$ and $g(\Gamma) = n - 1$. Figure 3 shows an example. Using the same notation for the corresponding simple pm-graph, we obtain the results given in the tables below:

We used Mathematica [19] to do the symbolic computations given in Tables 2, 3 and 4. As the number of vertices gets larger the expressions in the results become more complicated, so we listed the results only for small values of n . Again we used Mathematica [19] to do exact computations given in Table 5.

FIGURE 3. Ladder graph $L_3(a, b)$.

n	e	v	$g(L_n(a, b))$	$\ell(L_n(a, b))$
2	4	4	1	$2(a + b)$
3	7	6	2	$4a + 3b$
4	10	8	3	$2(3a + 2b)$
5	13	10	4	$8a + 5b$

TABLE 1. Number of edges, vertices, genus and length of $L_n(a, b)$ for $n \in \{2, 3, 4, 5\}$.

n	$\frac{\tau(\Gamma)}{\ell(\Gamma)}$	$\frac{\theta(\Gamma)}{\ell(\Gamma)}$
2	$\frac{1}{12}$	0
3	$\frac{8a^2+14ab+7b^2}{12(2a+3b)(4a+3b)}$	$\frac{2b(2a+b)}{(2a+3b)(4a+3b)}$
4	$\frac{12a^4+36a^3b+38a^2b^2+18ab^3+3b^4}{24(a+b)(3a+2b)(2a^2+4ab+b^2)}$	$\frac{4a^4+20a^3b+26a^2b^2+10ab^3+b^4}{(a+b)(3a+2b)(2a^2+4ab+b^2)}$
5	$\frac{128a^5+496a^4b+704a^3b^2+476a^2b^3+160ab^4+19b^5}{12(8a+5b)(4a^2+6ab+b^2)(4a^2+10ab+5b^2)}$	$\frac{2(128a^5+656a^4b+1104a^3b^2+716a^2b^3+160ab^4+9b^5)}{(8a+5b)(4a^2+6ab+b^2)(4a^2+10ab+5b^2)}$

TABLE 2. For pm-graph $\Gamma = L_n(a, b)$, $\tau(\Gamma)$ and $\theta(\Gamma)$ for $n \in \{2, 3, 4, 5\}$.

n	$\frac{\varphi(\Gamma)}{\ell(\Gamma)}$	$\frac{\lambda(\Gamma)}{\ell(\Gamma)}$
2	0	$\frac{1}{12}$
3	$\frac{2a^2+2ab+b^2}{3(2a+3b)(4a+3b)}$	$\frac{1}{10}$
4	$\frac{72a^4+192a^3b+164a^2b^2+60ab^3+9b^4}{72(a+b)(3a+2b)(2a^2+4ab+b^2)}$	$\frac{5a+3b}{14(3a+2b)}$
5	$\frac{(2a+b)(16a^4+52a^3b+51a^2b^2+16ab^3+2b^4)}{(8a+5b)(4a^2+6ab+b^2)(4a^2+10ab+5b^2)}$	$\frac{5(2a+b)}{9(8a+5b)}$

TABLE 3. For pm-graph $\Gamma = L_n(a, b)$, $\varphi(\Gamma)$ and $\lambda(\Gamma)$ for $n \in \{2, 3, 4, 5\}$.

n	$\frac{\epsilon(\Gamma)}{\ell(\Gamma)}$	$\frac{Z(\Gamma)}{\ell(\Gamma)}$
2	0	$\frac{1}{12}$
3	$\frac{4a^2+10ab+5b^2}{3(2a+3b)(4a+3b)}$	$\frac{(a+b)^2}{2(2a+3b)(4a+3b)}$
4	$\frac{36a^4+132a^3b+154a^2b^2+66ab^3+9b^4}{18(a+b)(3a+2b)(2a^2+4ab+b^2)}$	$\frac{36a^4+120a^3b+134a^2b^2+60ab^3+9b^4}{108(a+b)(3a+2b)(2a^2+4ab+b^2)}$
5	$\frac{64a^5+288a^4b+452a^3b^2+298a^2b^3+80ab^4+7b^5}{(8a+5b)(4a^2+6ab+b^2)(4a^2+10ab+5b^2)}$	$\frac{5(2a+b)(16a^4+60a^3b+73a^2b^2+32ab^3+4b^4)}{24(8a+5b)(4a^2+6ab+b^2)(4a^2+10ab+5b^2)}$

TABLE 4. For pm-graph $\Gamma = L_n(a, b)$, $\epsilon(\Gamma)$ and $Z(\Gamma)$ for $n \in \{2, 3, 4, 5\}$.

n	$\frac{\tau(\Gamma)}{\ell(\Gamma)}$	$\frac{\theta(\Gamma)}{\ell(\Gamma)}$	$\frac{\varphi(\Gamma)}{\ell(\Gamma)}$	$\frac{\lambda(\Gamma)}{\ell(\Gamma)}$	$\frac{\epsilon(\Gamma)}{\ell(\Gamma)}$	$\frac{Z(\Gamma)}{\ell(\Gamma)}$
5	$\frac{661}{10868}$	$\frac{5546}{2717}$	$\frac{411}{2717}$	$\frac{5}{39}$	$\frac{1189}{2717}$	$\frac{925}{21736}$
10	$\frac{2107}{37829}$	$\frac{554308}{37829}$	$\frac{30329}{71676}$	$\frac{15}{76}$	$\frac{344578}{340461}$	$\frac{210215}{6128298}$
15	$\frac{3061011619}{56529128700}$	$\frac{180955287578}{4710760725}$	$\frac{2384321993}{3411240525}$	$\frac{665}{2494}$	$\frac{155613041207}{98925975225}$	$\frac{2950668709}{92330910210}$
20	$\frac{105284865781}{1971566979888}$	$\frac{6020905705851}{82148624162}$	$\frac{12183994532757}{12486590872624}$	$\frac{380}{1131}$	$\frac{6652614900537}{3121647718156}$	$\frac{10979128575725}{355867839869784}$

TABLE 5. For pm-graph $\Gamma = L_n(1, 1)$, computations of $\tau(\Gamma)$, $\theta(\Gamma)$, $\varphi(\Gamma)$, $\lambda(\Gamma)$, $\epsilon(\Gamma)$ and $Z(\Gamma)$ when $n \in \{5, 10, 15, 20\}$.

n	$\frac{\tau(\Gamma)}{\ell(\Gamma)}$	$\frac{\theta(\Gamma)}{\ell(\Gamma)}$	$\frac{\varphi(\Gamma)}{\ell(\Gamma)}$	$\frac{\lambda(\Gamma)}{\ell(\Gamma)}$	$\frac{\epsilon(\Gamma)}{\ell(\Gamma)}$	$\frac{Z(\Gamma)}{\ell(\Gamma)}$
500	0.05134130	55155.801168	27.6397	7.00233	55.4713	0.0278941
1000	0.05129978	221422.325273	55.4174	13.9468	111.027	0.0278359
5000	0.05126659	5551550.777737	277.639	69.5023	555.471	0.0277894
10000	0.05126245	22214198.121181	555.417	138.947	1111.03	0.0277836
15000	0.05126107	49987945.991478	833.194	208.391	1666.58	0.0277816
20000	0.05126038	88872829.563811	1110.97	277.835	2222.14	0.0277807
25000	0.05125992	138868444.360781	1388.75	347.279	2777.69	0.02778

TABLE 6. For pm-graph $\Gamma = L_n(1, 1)$, computations of $\tau(\Gamma)$, $\theta(\Gamma)$, $\varphi(\Gamma)$, $\lambda(\Gamma)$, $\epsilon(\Gamma)$ and $Z(\Gamma)$ when $n \in \{500, 1000, 10000, 15000, 20000, 25000\}$.

Finally, we used Matlab [16], which does machine arithmetic, to obtain the results in Table 6. Note that when $n = 25000$ in Table 6, $L_n(1, 1)$ has 50000 vertices and 75000 – 2 edges. As such computations would be possible on a computer with high memory and processing speed, we used Mac Pro with processor 2×2.93 GHz 6-core Intel Xeon (24 hyper-threading in total) and memory 32 GB 1333 MHz DDR3 to obtain these results.

Symbolic computations are clearly the most costly computations. Among the numerical computations, we can have exact arithmetic (arithmetic with numbers having an infinite number of significant figures, i.e, with numbers having infinite precision), precision arithmetic (which involves the numbers with precision more than 18) and arithmetic with machine numbers.

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ZUBEYIR CINKIR, DEPARTMENT OF MATHEMATICS, ZIRVE UNIVERSITY, 27260, GAZIANTEP, TURKEY,
E-mail address: `zubeyir.cinkir@zirve.edu.tr`